

Auramine
492-80-8 | DTXSID7043821

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 349 °C

Global applicability domain: Outside

Local applicability domain index: 2.94e-01

Confidence level: 4.91e-01

Nearest Neighbors from the Training Set

Image not found

Auramine

Measured: 331

Predicted: 349

Image not found

4-Aminoazobenzene

Measured: 366

Predicted: 337

Image not found

Pendimethalin

Measured: 330

Predicted: 335

Image not found

Dehydrothio-4-toluidine

Measured: 434

Predicted: 377

Image not found

3-Methyl-1-phenyl-1H-pyrazol-5-amine

Measured: 333

Predicted: 334